

Supplementary data for article:

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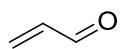
## Supporting Information

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### **Electron Delocalization in Electron-Deficient Alkenes and Push-Pull Alkenes**

Zdravko Džambaski and Marija Baranac-Stojanović\*

# Absolute energies (a.u.) and x,y,z coordinates (Å) of optimized structures



**4a-s-trans**

E = -191.9741857 a.u.

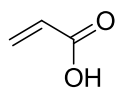
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.207008	1.290216	0.000000
2	6	0	0.000000	0.718937	0.000000
3	6	0	-0.147986	-0.747609	0.000000
4	8	0	-1.211570	-1.326134	0.000000
5	1	0	1.336300	2.366037	0.000000
6	1	0	2.111289	0.688157	0.000000
7	1	0	-0.917487	1.299201	0.000000
8	1	0	0.808323	-1.313584	0.000000



**4a-s-cis**

E = -191.9707324 a.u.

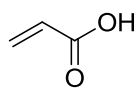
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.330969	0.789453	0.000000
2	6	0	0.000000	0.893209	0.000000
3	6	0	-0.885656	-0.298528	0.000000
4	8	0	-0.498110	-1.445973	0.000000
5	1	0	1.971234	1.663720	0.000000
6	1	0	1.804856	-0.186377	0.000000
7	1	0	-0.490717	1.862419	0.000000
8	1	0	-1.972367	-0.076783	0.000000



**4b-s-trans**

E = -267.2525696 a.u.

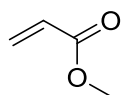
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.300896	-1.903864	0.000000
2	6	0	-0.809562	-0.672226	0.000000
3	6	0	0.000000	0.566153	0.000000
4	8	0	-0.470542	1.680108	0.000000
5	8	0	1.339550	0.343396	0.000000
6	1	0	-0.947493	-2.774013	0.000000
7	1	0	0.768799	-2.074982	0.000000
8	1	0	-1.878057	-0.491561	0.000000
9	1	0	1.767434	1.212142	0.000000



**4b-s-cis**

E = -267.2531306 a.u.

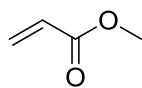
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.436674	-1.922893	0.000000
2	6	0	-0.446594	-0.926312	0.000000
3	6	0	0.000000	0.487775	0.000000
4	8	0	-1.060735	1.336112	0.000000
5	8	0	1.143268	0.877277	0.000000
6	1	0	0.118877	-2.958644	0.000000
7	1	0	1.501281	-1.716693	0.000000
8	1	0	-1.516086	-1.100434	0.000000
9	1	0	-0.704819	2.237241	0.000000



**4c-s-trans**

E = -306.5625362 a.u.

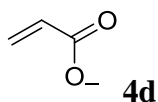
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.170106	-0.772012	0.000093
2	6	0	-1.492957	0.375510	-0.000020
3	6	0	-0.014130	0.486620	-0.000100
4	8	0	0.574945	1.544088	0.000056
5	8	0	0.610578	-0.711014	-0.000254
6	6	0	2.048485	-0.669280	0.000144
7	1	0	-3.254142	-0.779735	0.000165
8	1	0	-1.661423	-1.728304	0.000112
9	1	0	-1.996127	1.335650	-0.000034
10	1	0	2.368807	-1.708900	0.003348
11	1	0	2.415205	-0.151421	0.887509
12	1	0	2.415757	-0.156914	-0.890216



**4c-s-cis**

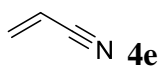
E = -306.5635607 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.494442	-0.018867	-0.000018
2	6	0	1.317732	-0.642216	-0.000007
3	6	0	0.045497	0.123331	0.000049
4	8	0	-0.059283	1.327890	0.000000
5	8	0	-1.014187	-0.717186	0.000042
6	6	0	-2.311084	-0.094546	-0.000043
7	1	0	3.426500	-0.571287	-0.000054
8	1	0	2.544131	1.064395	0.000012
9	1	0	1.235559	-1.722794	-0.000030
10	1	0	-3.026729	-0.913638	-0.001269
11	1	0	-2.435131	0.526689	-0.888204
12	1	0	-2.436102	0.524783	0.889328



E = -266.6959716 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.183374	-1.910422	0.000000
2	6	0	-0.564169	-0.805785	0.000000
3	6	0	0.000000	0.626912	0.000000
4	8	0	-0.882855	1.523972	0.000000
5	8	0	1.248090	0.743216	0.000000
6	1	0	-0.251231	-2.908338	0.000000
7	1	0	1.265762	-1.819795	0.000000
8	1	0	-1.651641	-0.873603	0.000000



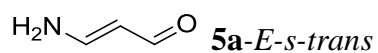
E = -170.8828756 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.317580	-0.985412	0.000000
2	6	0	0.000000	-0.769923	0.000000
3	6	0	0.577096	0.535979	0.000000
4	7	0	1.068231	1.582095	0.000000
5	1	0	-1.710234	-1.994668	0.000000
6	1	0	-2.029562	-0.169006	0.000000
7	1	0	0.705086	-1.594850	0.000000



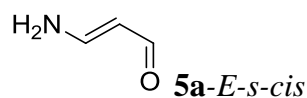
E = -283.1790511 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.157611	-1.866219	0.000000
2	6	0	-0.600684	-0.781971	0.000000
3	7	0	0.000000	0.562563	0.000000
4	8	0	-0.793073	1.497363	0.000000
5	8	0	1.218153	0.668512	0.000000
6	1	0	-0.300108	-2.847263	0.000000
7	1	0	1.237551	-1.789930	0.000000
8	1	0	-1.679642	-0.738609	0.000000



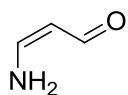
E = -247.3635528 a.u.; 33.91i cm<sup>-1</sup>

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.977220	-0.570326	0.000000
2	6	0	0.000000	0.368513	0.000000
3	6	0	-1.389199	-0.034968	0.000000
4	8	0	-2.347241	0.718400	0.000000
5	7	0	2.316623	-0.352094	0.000000
6	1	0	0.698494	-1.621179	0.000000
7	1	0	0.222286	1.431113	0.000000
8	1	0	-1.549625	-1.137750	0.000000
9	1	0	2.969022	-1.115516	0.000000
10	1	0	2.693263	0.581470	0.000000



E = -247.3620593 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.847090	-0.338215	0.000000
2	6	0	0.000000	0.722004	0.000000
3	6	0	-1.438280	0.511676	0.000000
4	8	0	-2.005234	-0.570853	0.000000
5	7	0	2.200297	-0.298674	0.000000
6	1	0	0.414868	-1.334573	0.000000
7	1	0	0.368462	1.743314	0.000000
8	1	0	-2.039741	1.444776	0.000000
9	1	0	2.743051	-1.144103	0.000000
10	1	0	2.700299	0.575341	0.000000



**5a-Z-s-trans**

E = -247.358422 a.u.; 95.69i cm<sup>-1</sup>

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.300001	0.345845	0.000000
2	6	0	0.000000	0.747587	0.000000
3	6	0	1.144182	-0.135809	0.000000
4	7	0	-1.799344	-0.918972	0.000000
5	8	0	2.309086	0.225135	0.000000
6	1	0	-2.073358	1.108052	0.000000
7	1	0	0.204261	1.811077	0.000000
8	1	0	0.923136	-1.228484	0.000000
9	1	0	-2.791223	-1.074434	0.000000
10	1	0	-1.205191	-1.730228	0.000000

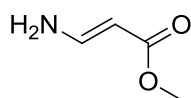


**5a-Z-s-cis**

E = -247.3700201 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.189435	0.414197	0.000000
2	6	0	0.000000	1.096384	0.000000
3	6	0	-1.266119	0.418277	0.000000
4	7	0	1.303694	-0.924314	0.000000
5	8	0	-1.411872	-0.808677	0.000000
6	1	0	2.126995	0.962677	0.000000
7	1	0	0.016548	2.178097	0.000000
8	1	0	-2.162992	1.066756	0.000000
9	1	0	2.203426	-1.371927	0.000000
10	1	0	0.445248	-1.469147	0.000000

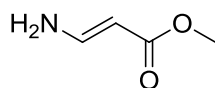




**5b-E-s-trans**

E = -361.9496652 a.u.; 177.45i cm<sup>-1</sup>

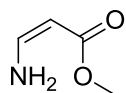
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.686581	-0.383161	-0.000036
2	6	0	-0.846809	0.676100	-0.000017
3	6	0	0.603823	0.553149	0.000005
4	7	0	-3.045666	-0.326370	-0.000058
5	8	0	1.376204	1.490536	0.000034
6	8	0	1.038252	-0.743714	0.000019
7	6	0	2.461422	-0.921185	0.000048
8	1	0	-1.275844	-1.386521	-0.000035
9	1	0	-1.216424	1.694944	-0.000016
10	1	0	-3.598775	-1.163971	-0.000072
11	1	0	-3.533068	0.554212	-0.000062
12	1	0	2.621210	-1.998117	-0.000070
13	1	0	2.907860	-0.470081	0.887996
14	1	0	2.907925	-0.469871	-0.887759



**5b-E-s-cis**

E = -361.951325 a.u.; 141.25i cm<sup>-1</sup>

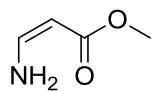
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.896711	0.239310	-0.000023
2	6	0	0.770309	-0.506986	-0.000032
3	7	0	3.174842	-0.221075	-0.000057
4	6	0	-0.526797	0.157288	0.000008
5	8	0	-1.539869	-0.754688	0.000003
6	8	0	-0.731966	1.356348	0.000053
7	6	0	-2.867527	-0.211752	0.000044
8	1	0	1.797143	1.320307	0.000014
9	1	0	0.790867	-1.590005	-0.000068
10	1	0	3.952250	0.414045	-0.000046
11	1	0	3.377913	-1.206730	-0.000093
12	1	0	-3.534455	-1.071997	-0.000089
13	1	0	-3.034573	0.400608	0.888016
14	1	0	-3.034530	0.400854	-0.887765



**5b-Z-s-trans**

E = -361.9523953 a.u.

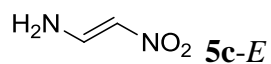
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.979230	0.300616	-0.000098
2	6	0	-0.876991	1.096905	-0.000031
3	6	0	0.514240	0.680129	0.000112
4	8	0	1.473079	1.422817	0.000051
5	7	0	-2.041043	-1.051570	-0.000046
6	8	0	0.671022	-0.691423	0.000031
7	6	0	2.031145	-1.157437	0.000014
8	1	0	-2.950597	0.786052	-0.000201
9	1	0	-1.022127	2.167520	-0.000092
10	1	0	-2.926436	-1.524195	-0.000106
11	1	0	-1.185897	-1.586502	0.000056
12	1	0	1.969729	-2.244496	-0.000144
13	1	0	2.557382	-0.805042	0.888085
14	1	0	2.557453	-0.804786	-0.887912



**5b-Z-s-cis**

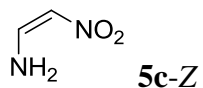
E = -361.9574131 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.021892	0.610047	-0.000032
2	6	0	-0.720402	1.013215	-0.000061
3	6	0	0.366322	0.059601	-0.000053
4	8	0	1.583935	0.660761	-0.000011
5	8	0	0.247024	-1.161681	0.000045
6	7	0	-2.460499	-0.666513	0.000000
7	6	0	2.718990	-0.216792	0.000072
8	1	0	-2.803804	1.363189	-0.000039
9	1	0	-0.488036	2.067627	-0.000089
10	1	0	-3.442017	-0.877202	0.000020
11	1	0	-1.773166	-1.410842	0.000003
12	1	0	3.590022	0.435698	-0.000035
13	1	0	2.717382	-0.850857	0.888426
14	1	0	2.717329	-0.851095	-0.888111



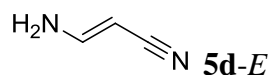
E = -338.5680149 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.288753	0.188194	0.000000
2	6	0	0.000000	0.590464	0.000000
3	7	0	2.372012	0.996954	0.000000
4	7	0	-1.048017	-0.385310	0.000000
5	8	0	-2.201327	0.049646	0.000000
6	8	0	-0.763659	-1.586611	0.000000
7	1	0	1.489370	-0.877138	0.000000
8	1	0	-0.355185	1.609095	0.000000
9	1	0	3.299101	0.610123	0.000000
10	1	0	2.286115	2.000182	0.000000



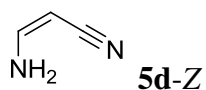
E = -338.5748102 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.615362	-1.411755	0.000000
2	6	0	0.954882	-0.092476	0.000000
3	7	0	-0.611830	-1.951920	0.000000
4	7	0	0.000000	0.953775	0.000000
5	8	0	0.412211	2.112646	0.000000
6	8	0	-1.213437	0.658354	0.000000
7	1	0	1.437866	-2.119343	0.000000
8	1	0	1.977851	0.243242	0.000000
9	1	0	-0.733481	-2.949427	0.000000
10	1	0	-1.411079	-1.330071	0.000000



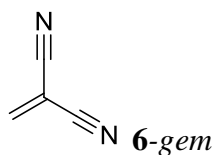
E = -226.2695925 a.u.; 178.69i cm<sup>-1</sup>

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.821456	-0.536663	0.000000
2	6	0	0.000000	0.539262	0.000000
3	6	0	1.407442	0.396839	0.000000
4	7	0	-2.180127	-0.504638	0.000000
5	7	0	2.562401	0.301155	0.000000
6	1	0	-0.395377	-1.534197	0.000000
7	1	0	-0.394403	1.550001	0.000000
8	1	0	-2.715928	-1.353409	0.000000
9	1	0	-2.686124	0.365357	0.000000



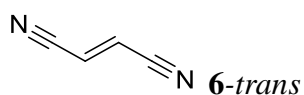
E = -226.2725243 a.u.; 72.63i cm<sup>-1</sup>

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.210251	0.369857	0.000000
2	6	0	0.000000	0.983833	0.000000
3	6	0	1.202938	0.240278	0.000000
4	7	0	-1.431464	-0.967656	0.000000
5	7	0	2.162798	-0.410443	0.000000
6	1	0	-2.107023	0.979296	0.000000
7	1	0	0.057702	2.062638	0.000000
8	1	0	-2.363870	-1.339101	0.000000
9	1	0	-0.662270	-1.619951	0.000000



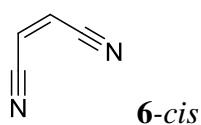
E = -263.1370413 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000003	1.745529	0.000000
2	6	0	0.000000	0.402823	0.000000
3	6	0	-1.222674	-0.349369	0.000000
4	6	0	1.222672	-0.349373	0.000000
5	7	0	-2.208234	-0.949571	0.000000
6	7	0	2.208232	-0.949575	0.000000
7	1	0	0.930445	2.298179	0.000000
8	1	0	-0.930436	2.298183	0.000000



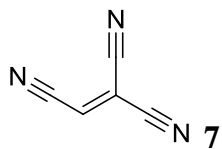
E = -263.1442894 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.333022	0.583349	0.000000
2	6	0	0.333022	-0.583349	0.000000
3	6	0	-0.333022	-1.840076	0.000000
4	6	0	0.333022	1.840076	0.000000
5	7	0	-0.848405	-2.874319	0.000000
6	7	0	0.848405	2.874319	0.000000
7	1	0	-1.417345	0.609208	0.000000
8	1	0	1.417345	-0.609208	0.000000



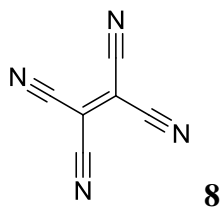
E = -263.1424984 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.127513	0.503439	0.000000
2	6	0	0.000000	1.234732	0.000000
3	6	0	1.315255	0.694190	0.000000
4	6	0	-1.170311	-0.917918	0.000000
5	7	0	2.400344	0.297475	0.000000
6	7	0	-1.250086	-2.070496	0.000000
7	1	0	-2.087471	1.007640	0.000000
8	1	0	-0.068924	2.316855	0.000000



E = -355.3926706 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.095032	-0.317541	0.000000
2	6	0	0.000000	0.479069	0.000000
3	6	0	0.145409	1.902994	0.000000
4	6	0	-1.334617	-0.035063	0.000000
5	6	0	1.041714	-1.733230	0.000000
6	7	0	0.261892	3.051257	0.000000
7	7	0	-2.416888	-0.435505	0.000000
8	7	0	1.045588	-2.888875	0.000000
9	1	0	2.080638	0.134491	0.000000



E = -447.6380977 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.683847	0.000000
2	6	0	0.000000	-0.683847	0.000000
3	6	0	1.215260	-1.430922	0.000000
4	6	0	-1.215259	-1.430924	0.000000
5	6	0	-1.215260	1.430922	0.000000
6	6	0	1.215259	1.430924	0.000000
7	7	0	2.186653	-2.054786	0.000000
8	7	0	-2.186653	-2.054785	0.000000
9	7	0	-2.186653	2.054786	0.000000
10	7	0	2.186653	2.054785	0.000000